```
Welcome to STN International
NEWS
                 Web Page URLs for STN Seminar Schedule - N. America
NEWS
                  "Ask CAS" for self-help around the clock
NEWS
                 New e-mail delivery for search results now available
         Jun 03
NEWS
      4
         Aug 08
                 PHARMAMarketLetter(PHARMAML) - new on STN
                 Aquatic Toxicity Information Retrieval (AQUIRE)
NEWS
         Aug 19
                 now available on STN
NEWS
      6
         Aug 26
                 Sequence searching in REGISTRY enhanced
      7
NEWS
         Sep 03
                 JAPIO has been reloaded and enhanced
NEWS
                 Experimental properties added to the REGISTRY file
         Sep 16
                 CA Section Thesaurus available in CAPLUS and CA
NEWS
         Sep 16
NEWS 10
         Oct 01
                 CASREACT Enriched with Reactions from 1907 to 1985
NEWS 11
         Oct 24
                 BEILSTEIN adds new search fields
NEWS 12 Oct 24
                 Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 13 Nov 18 DKILIT has been renamed APOLLIT
NEWS 14 Nov 25
                 More calculated properties added to REGISTRY
NEWS 15 Dec 04 CSA files on STN .
NEWS 16 Dec 17
                 PCTFULL now covers WP/PCT Applications from 1978 to date
NEWS 17 Dec 17
                 TOXCENTER enhanced with additional content
NEWS 18 Dec 17
                 Adis Clinical Trials Insight now available on STN
NEWS 19 Jan 29
                 Simultaneous left and right truncation added to COMPENDEX,
                 ENERGY, INSPEC
                 CANCERLIT is no longer being updated
NEWS 20
         Feb 13
NEWS 21
         Feb 24
                 METADEX enhancements
NEWS 22
                 PCTGEN now available on STN
         Feb 24
NEWS 23 Feb 24
                 TEMA now available on STN
NEWS 24 Feb 26
                 NTIS now allows simultaneous left and right truncation
NEWS 25 Feb 26 PCTFULL now contains images
NEWS 26 Mar 04
                 SDI PACKAGE for monthly delivery of multifile SDI results
NEWS 27 Mar 20 EVENTLINE will be removed from STN
NEWS 28 Mar 24
                 PATDPAFULL now available on STN
NEWS 29 Mar 24
                 Additional information for trade-named substances without
                 structures available in REGISTRY
NEWS 30
        Apr 11 Display formats in DGENE enhanced
NEWS 31
         Apr 14 MEDLINE Reload
NEWS 32
         Apr 17
                 Polymer searching in REGISTRY enhanced
NEWS 33
                 Indexing from 1947 to 1956 added to records in CA/CAPLUS
         Jun 13
NEWS 34
         Apr 21
                 New current-awareness alert (SDI) frequency in
                 WPIDS/WPINDEX/WPIX
NEWS 35
         Apr 28
                 RDISCLOSURE now available on STN
NEWS 36
         May 05 Pharmacokinetic information and systematic chemical names
                 added to PHAR
NEWS 37
         May 15
                 MEDLINE file segment of TOXCENTER reloaded
NEWS 38
         May 15
                 Supporter information for ENCOMPPAT and ENCOMPLIT updated
NEWS 39
         May 16
                 CHEMREACT will be removed from STN
NEWS 40
         May 19
                 Simultaneous left and right truncation added to WSCA
NEWS 41
        May 19
                 RAPRA enhanced with new search field, simultaneous left and
                 right truncation
NEWS 42
         Jun 06
                 Simultaneous left and right truncation added to CBNB
NEWS 43
         Jun 06
                 PASCAL enhanced with additional data
NEWS 44
         Jun 20
                 2003 edition of the FSTA Thesaurus is now available
NEWS 45
        Jun 25 HSDB has been reloaded
NEWS EXPRESS April 4 CURRENT WINDOWS VERSION IS V6.01a, CURRENT
              MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP),
              AND CURRENT DISCOVER FILE IS DATED 01 APRIL 2003
NEWS HOURS
              STN Operating Hours Plus Help Desk Availability
NEWS INTER
              General Internet Information
NEWS LOGIN
             Welcome Banner and News Items
```

NEWS PHONE Direct Dial and Telecommunication Network Access to STN NEWS WWW CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 05:20:39 ON 30 JUN 2003

=> file req

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 0.21 0.21

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STRUCTURE FILE UPDATES: 27 JUN 2003 HIGHEST RN 539020-41-2 DICTIONARY FILE UPDATES: 27 JUN 2003 HIGHEST RN 539020-41-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> e nicotinamide/cn

El	1	NICOTINAMIDASE/ PYRAZINAMIDASE (SALMONELLA ENTERICA TYPHIMUR
		IUM STRAIN LT2; SGSC 1412; ATCC 700720 GENE PNCA)/CN
E2	1	NICOTINAMIDASE/PYRAZINAMIDASE (PSEUDOMONAS STRAIN ADP GENE A
		TZE)/CN
E3	1>	NICOTINAMIDE/CN
E4	1	NICOTINAMIDE (5-(BROMOACETYL)-4-METHYLIMIDAZOLE) DINUCLEOTID
		E/CN
E5	1	NICOTINAMIDE 1, N6-ETHENOADENINE DINUCLEOTIDE/CN
E6	1	NICOTINAMIDE 1, N6-ETHENOADENINE DINUCLEOTIDE PHOSPHATE/CN
E7	1	NICOTINAMIDE 2'-DEOXYADENOSINE DINUCLEOTIDE/CN
E8	·1	NICOTINAMIDE 2'-DEOXYADENOSINE DINUCLEOTIDE, REDUCED/CN
E9	1	NICOTINAMIDE 2-AMINO-4- (METHOXYMETHYL) -6-METHYL-/CN
E10	1	NICOTINAMIDE 2-AMINOPURINE RIBOSIDE DINUCLEOTIDE/CN
E11	1	NICOTINAMIDE 3, N4-ETHENOCYTOSINE DINUCLEOTIDE/CN
E12	1	NICOTINAMIDE 3-DEAZAPURINE DINUCLEOTIDE/CN

```
=> 8 e3
             1 NICOTINAMIDE/CN
L1
=> d 11
     ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS
L1
RN
     98-92-0 REGISTRY
CN
     3-Pyridinecarboxamide (9CI)
                                   (CA INDEX NAME)
OTHER CA INDEX NAMES:
     Nicotinamide (8CI)
OTHER NAMES:
CN
     β-Pyridinecarboxamide
     3-(Aminocarbonyl)pyridine
CN
CN
     3-Amidopyridine
CN
     3-Carbamoylpyridine
CN
     3-Pyridinecarboxylic acid amide
CN
     Aminicotin
CN
     Benicot
CN
     Delonin Amide
CN
     Dipegyl
CN
     m-(Aminocarbonyl)pyridine
CN
     NAM
CN .
     Niacinamide
CN
     Niavit PP
     Nicamina
CN
CN
     Nicamindon
CN
     Nicasir
CN
     Nicobion
CN
     Nicofort
CN
     Nicosan 2
     Nicosylamide
CN.
     Nicotilamide
CN
CN
     Nicotine acid amide
CN
     Nicotinic acid amide
CN
     Nicotinic amide
CN
     Nicotylamide
CN
     Nicovit
     Nicovitina
CN
CN
     Nictoamide
CN
     Niocinamide
CN
     Niozymin
CN
     Papulex
CN
     Pelmin
CN
     Pelmine
CN
     Pelonin amide
CN
     Vi-Nicotyl
CN
     Vitamin B
CN
     Vitamin B3
FS
     3D CONCORD
DR
     123574-63-0, 37321-14-5, 78731-47-2
MF
     C6 H6 N2 O
CI
     COM
LC
     STN Files:
                  ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*,
       BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS,
       CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM,
       CSNB, DDFU, DETHERM*, DIOGENES, DRUGU, EMBASE, GMELIN*, HODOC*, HSDB*,
       IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NAPRALERT,
       NIOSHTIC, PDLCOM*, PHAR, PIRA, PROMT, RTECS*, SPECINFO, TOXCENTER, USAN,
       USPAT2, USPATFULL, VTB
```

(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**, WHO
 (**Enter CHEMLIST File for up-to-date regulatory information)

```
C-NH<sub>2</sub>
```

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

7618 REFERENCES IN FILE CA (1957 TO DATE)
267 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
7620 REFERENCES IN FILE CAPLUS (1957 TO DATE)
9 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

```
=> e cyanopyridine/cn
            1
                  CYANOPTERINE/CN
            1
                  CYANOPYRAZINE/CN
            1 ---> CYANOPYRIDINE/CN
E3
E4
                 CYANOPYRIDINIUM BROMIDE/CN
            1
E5
            1
                  CYANOQUINONAMINE/CN
E6
            1
                  CYANORESIN CR-C/CN
E7
                  CYANORESIN CR-E/CN
E8
                 CYANORESIN CR-E TRIFLUOROMETHYLBENZOATE/CN
            1
                CYANORESIN CR-M/CN
E9
            1
E10
            1
                CYANORESIN CR-S/CN
E11
           1 CYANORESIN CR-S BENZOATE/CN
E12
                 , CYANORESIN CR-S FLUOROBENZOATE/CN
           1
=> s e3
L2
            1 CYANOPYRIDINE/CN
```

=> d 12

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS

RN 29386-66-1 REGISTRY

CN Pyridinecarbonitrile (6CI, 8CI, 9CI) (CA INDEX NAME)

OTHER NAMES:

CN Cyanopyridine

MF C6 H4 N2

CI IDS

LC STN Files: BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CIN, PROMT, TOXCENTER, USPAT2, USPATFULL



D1-CN

- 65 REFERENCES IN FILE CA (1957 TO DATE)
- 6 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
- 65 REFERENCES IN FILE CAPLUS (1957 TO DATE)

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

```
=>
         STRUCTURE UPLOADED
L3
=> d 13
L3 HAS NO ANSWERS
L3
                 STR
 63
VPA 7-2/3/4 S
NODE ATTRIBUTES:
NSPEC
        IS R
                  AΤ
                        1
NSPEC
        IS R
                   AT
NSPEC
        IS R
                   ΑT
NSPEC
        IS R
                   AΤ
NSPEC
        IS R
                   AT
                        5
NSPEC
        IS R
                   AT
NSPEC
        IS C
                   ΑT
NSPEC
        IS C
                  AT
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT
DEFAULT ECLEVEL IS LIMITED
GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS
STEREO ATTRIBUTES: NONE
=> s 13
SAMPLE SEARCH INITIATED 05:24:52 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -
                                    5903 TO ITERATE
 16.9% PROCESSED
                    1000 ITERATIONS
                                                                50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS:
                        ONLINE
                                 **COMPLETE**
                                 **COMPLETE**
                        BATCH
PROJECTED ITERATIONS:
                            113456 TO
                                         122664
PROJECTED ANSWERS:
                              32894 TO
                                         37942
L4
             50 SEA SSS SAM L3
```

=> s 13 full

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 147.75 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 05:25:06 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 118278 TO ITERATE

100.0% PROCESSED. 118278 ITERATIONS

34801 ANSWERS

SEARCH TIME: 00.00.01

L5 34801 SEA SSS FUL L3

=> L6

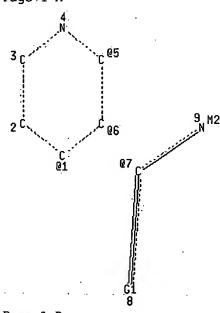
STRUCTURE UPLOADED

=> d 16

L6 HAS NO ANSWERS

L6

0 10 S 11 Page . 1 - A



Page 1-B VAR G1=10/11 VPA 7-1/5/6 S NODE ATTRIBUTES: HCOUNT IS M2 AT 9 NSPEC IS R AT 1 NSPEC IS R AT. NSPEC IS R AT NSPEC IS R AT 4 **NSPEC** IS R AT 5 **NSPEC** IS R AT NSPEC IS C AT 7 NSPEC IS C AT 8 NSPEC IS C AT DEFAULT MLEVEL IS ATOM MLEVEL IS CLASS AT 9 10 11 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 11

STEREO ATTRIBUTES: NONE

=> s 16

SAMPLE SEARCH INITIATED 05:26:53 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 27967 TO ITERATE

3.6% PROCESSED 1000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

18 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 549361 TO 569319 PROJECTED ANSWERS: 8722 TO 11414

L7 18 SEA SSS SAM L6

=> file hcaplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 163.95 164.16

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FILE COVERS 1907 - 30 Jun 2003 VOL 139 ISS 1 FILE LAST UPDATED: 29 Jun 2003 (20030629/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 05:20:39 ON 30 JUN 2003)

FILE 'REGISTRY' ENTERED AT 05:20:47 ON 30 JUN 2003

E NICOTINAMIDE/CN

L1 1 S E3

E CYANOPYRIDINE/CN

L2 1 S E3

L3 STRUCTURE UPLOADED

L4 50 S L3

L5 34801 S L3 FULL

L6 STRUCTURE UPLOADED

L7

18 S L6

FILE 'HCAPLUS' ENTERED AT 05:27:14 ON 30 JUN 2003

=> s 11/prep

7664 L1

3020723 PREP/RL

L8

250 L1/PREP

(L1 (L) PREP/RL)

=> s 15/rct

10933 L5

2532391 RCT/RL

L9

5151 L5/RCT

(L5 (L) RCT/RL)

=> s 19 and 18

80 L9 AND L8 L10

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

4.51 168.67

FILE 'REGISTRY' ENTERED AT 05:28:15 ON 30 JUN 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: 27 JUN 2003 HIGHEST RN 539020-41-2 DICTIONARY FILE UPDATES: 27 JUN 2003 HIGHEST RN 539020-41-2

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

water/cn			
1		WATCON	1255/CN
1		WATCON	130/CN
1	>	WATER/	'CN
1		WATER	((H2O)2)/CN
1		WATER	(D2180)/CN
1		WATER	(D2O1+)/CN
1		WATER	(DOT), HEAVY/CN
1		WATER	(DTO)/CN
1		WATER	(H170H)/CN
1		WATER	(H2140)/CN
1		WATER	(H2150)/CN
1		WATER	(H2170)/CN
	1 1 1 1 1 1 1 1	1 1 1> 1 1 1 1 1 1 1	1 WATCON 1 WATCON 1> WATER 1 WATER

=> s e3

L11

1 WATER/CN

=> d 111

L11 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2003 ACS

RN 7732-18-5 REGISTRY

CN Water (8CI, 9CI) (CA INDEX NAME)

OTHER NAMES:

CN 1593: PN: WO03025132 TABLE: 42 claimed sequence

CN Distilled water

CN DRIWATER

CN Hydrogen oxide (H2O)

CN R 718

FS 3D CONCORD

MF H2 O

CI COM

LC STN Files: ANABSTR, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAPLUS, CASREACT, CBNB, CHEMCATS, CHEMINFORMRX, CHEMLIST, CHEMSAFE, CSCHEM, CSNB, DETHERM*, DIPPR*, EMBASE, GMELIN*, IFICDB, IFIPAT, IFIUDB, IPA, MEDLINE, MRCK*, MSDS-OHS, NIOSHTIC, PDLCOM*, RTECS*, SPECINFO, TOXCENTER, ULIDAT, USAN, USPAT2, USPATFULL, VTB

(*File contains numerically searchable property data)
Other Sources: DSL**, EINECS**, TSCA**

(**Enter CHEMLIST File for up-to-date regulatory information)

H₂0

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

287130 REFERENCES IN FILE CA (1957 TO DATE)
955 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
287291 REFERENCES IN FILE CAPLUS (1957 TO DATE)

=> file-hcaplus COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY 6.30 SESSION

FULL ESTIMATED COST

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FILE COVERS 1907 - 30 Jun 2003 VOL 139 ISS 1

FILE LAST UPDATED: 29 Jun 2003 (20030629/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 05:20:39 ON 30 JUN 2003)

FILE 'REGISTRY' ENTERED AT 05:20:47 ON 30 JUN 2003

E NICOTINAMIDE/CN

L1 1 S E3

E CYANOPYRIDINE/CN

L2 1 S E3

L3 STRUCTURE UPLOADED

L4 . 50 S L3

L5 34801 S L3 FULL

L6 STRUCTURE UPLOADED

L7 18 S L6

FILE 'HCAPLUS' ENTERED AT 05:27:14 ON 30 JUN 2003

L8 250 S L1/PREP

L9 5151 S L5/RCT

. L10 80 S L9 AND L8

FILE 'REGISTRY' ENTERED AT 05:28:15 ON 30 JUN 2003

E WATER/CN

L11 1 S E3

FILE 'HCAPLUS' ENTERED AT 05:28:39 ON 30 JUN 2003

=> s l11/rct

287548 L11

2532391 RCT/RL

L12 21445 L11/RCT

(L11 (L) RCT/RL)

=> s 112 and 110

L13 0 L12 AND L10

=> s 110 and metal?

2062308 METAL?

L14 7 L10 AND METAL?

=> s 114 and catal?

1182962 CATAL?

L15 5 L14 AND CATAL?

=> d 115, ibib abs hitstr, 1-5

L15 ANSWER 1 OF 5 HCAPLUS COPYRIGHT 2003 ACS

Full Citing
Text References
ACCESSION NUMBER:

2003:98167 HCAPLUS

DOCUMENT NUMBER:

138:287778

TITLE:

Organometallic Chemistry in Aqueous Solution.
Hydration of Nitriles to Amides Catalyzed by a
Water-Soluble Molybdocene, (MeCp) 2Mo (OH) (H2O) +
Breno, Kerry L.; Pluth, Michael D.; Tyler, David R.

AUTHOR (S):

CORPORATE SOURCE:

Department of Chemistry, University of Oregon, Eugene,

OR, 97403, USA

SOURCE:

Organometallics (2003), 22(6), 1203-1211

CODEN: ORGND7; ISSN: 0276-7333

PUBLISHER:

American Chemical Society

DOCUMENT TYPE:

Journal

LANGUAGE:

English

 $[Cp'2Mo(\mu-OH)2MoCp'2]2+(1)$ $(Cp'=\eta5-CH3C5H4)$ is a precatalyst for the hydration of nitriles in aq. soln. under mild conditions (-80°). Among the nitriles hydrated were acetonitrile, isobutyronitrile, benzonitrile, 3-hydroxypropionitrile, 3-bromopropioamide, 4-cyanopyridine, succinonitrile, Me cyanoacetate, 2-methoxyacetonitrile, and acrylonitrile. Except in the case of 2-methoxyacetonitrile, hydrolysis of the resulting amide products did not occur. Hydration of the C:C double bond did not occur in acrylonitrile, but hydrolysis of ester and ether linkages did occur in nitriles contg. those functional groups. The apparent rate consts. and turnover frequencies of the catalytic reactions were detd. using an iterative. kinetics-fitting program. The rates and turnover frequencies are comparable to those reported for many homogeneous nitrile hydration catalysts described in the literature. In aq. soln., 1 is in equil. with [Cp'2Mo(OH)(H2O)]+ (2), and this monomer is proposed to be the active hydration catalyst. The hydration is proposed to occur by an intramol. attack of a hydroxide ligand on a coordinated nitrile. The hydration reaction is irreversibly inhibited by product and reversibly inhibited by substrate (nitrile).

IT 100-48-1, 4-Cyanopyridine

RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent) (hydration kinetics; kinetics of molybdocene catalyzed hydration of nitriles to amides in aq. soln.)

RN 100-48-1 HCAPLUS

CN 4-Pyridinecarbonitrile (9CI) (CA INDEX NAME) Q 10410.07

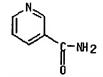


IT 98-92-0P, Nicotinamide

RL: SPN (Synthetic preparation); PREP (Preparation) (kinetics of molybdocene catalyzed hydration of nitriles to amides in aq. soln.)

RN 98-92-0 HCAPLUS

CN 3-Pyridinecarboxamide (9CI) (CA INDEX NAME)



REFERENCE COUNT:

THERE ARE 36 CITED REFERENCES AVAILABLE FOR THIS 36 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 2 OF 5 HCAPLUS COPYRIGHT 2003 ACS

Full Citing References ACCESSION NUMBER:

1996:431422 HCAPLUS

DOCUMENT NUMBER:

125:86507

TITLE:

Process and manganese dioxide-based catalysts for the preparation of nicotinamide via the hydration of

3-cyanopyridine

INVENTOR(S):

Eller, Karsten; Horn, Hans Christoph; Herion, Christof

PATENT ASSIGNEE(S):

BASF A.-G., Germany Ger. Offen., 4 pp.

SOURCE: CODEN: GWXXBX

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

P	ATENT	NO.		KI	ND	DATE			A	PPLI	CATI	ON NO	ο.	DATE				
				-:-					-									
<u>D1</u>	4440	927		A	1	1996	0523		D	E 19	94 - 4	4409	27	1994	1117			
W	9616	039		A	1	1996	0530		W	0 19	95-E	P440	9	1995	1109			
	₩:	AL,	AM,	AU,	BB,	BG,	BR,							GE,			JP.	
		KE,	KG,	KP,	KR,	KZ,	LK,	LR,	LS,	LT,	LV,	MD,	MG,	MK,	MN.	MW.	MX.	
		NO,	NZ,	PL,	RO,	RU,	SD,	SG,	SI,	SK,	TJ,	TM,	TT.	UA,	UG.	US.	UZ.	VN
	RW:	KE,	LS,	MW,	SD,	SZ,	UG,	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB.	GR.	IE.	• • •
		IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM.	GA,	GN.	ML.	MR.	
		NE,	SN,	TD,	TG						•	•	•			,	,	
<u>A</u> I	9538	717		A:	1 .	1996	0617		A	J 19	95-38	8717		1995	1109			
PRIORIT	Y APP	LN.	INFO	. :]	DE 1	994-4	1440	927		1994	1117			
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OTHER SOURCE(S):

CASREACT 125:86507

Nicotinamide is prepd. in high yield and selectivity by the hydration of 3-cyanopyridine in the presence of a mech. stabile catalyst comprising: (a) MnO2 30-95; (b) Al2O3 0.5-70, or SiO2, TiO2, or ZrO2 1-70; and (c) alkali metal oxides or alk. earth metal oxides 0.1-10%.

IT 98-92-0P, Nicotinamide

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(process and manganese dioxide-based catalysts for the prepn. of nicotinamide via the hydration of 3-cyanopyridine)

RN98-92-0 HCAPLUS

3-Pyridinecarboxamide (9CI) CN (CA INDEX NAME)



IT 100-54-9, 3-Cyanopyridine

RL: RCT (Reactant); RACT (Reactant or reagent) (process and manganese dioxide-based catalysts for the prepn. of nicotinamide via the hydration of 3-cyanopyridine)

RN 100-54-9 HCAPLUS

CN 3-Pyridinecarbonitrile (9CI) (CA INDEX NAME)



L15 ANSWER 3 OF 5 HCAPLUS COPYRIGHT 2003 ACS

Citing References Text

ACCESSION NUMBER:

1992:128194 HCAPLUS

DOCUMENT NUMBER:

116:128194

TITLE:

Process for the preparation of copper catalysts with

increased surface area

INVENTOR(S):

Marayti, Ravindranathan; Sivaram, Swaminathan

PATENT ASSIGNEE(S):

Indian Petrochemicals Corp. Ltd., India

SOURCE:

Indian, 31 pp.

CODEN: INXXAP

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
IN 166044 ·	· A	19900303	IN 1986-B0147	19860515
IN 168607	Α	19910504	IN 1989-B063	19890313
PRIORITY APPLN. INFO.	. :		IN 1986-B0147	19860515

OTHER SOURCE(S):

MARPAT 116:128194

The title process useful for conversions of partially water-sol. org. nitriles to the corresponding amides, comprises redn. at 0-40° of ≥1 higher valent Cu salts by controlled addn. of an aq. soln. of a reducing agent, such as metal borohydride or an aldehyde for 2-5 h. ratio of Cu salt-reducing agent is 0.5:1.8. After the reaction is complete, the catalyst is extd. and washed until the water evinces a pH 5.5-6. CuSO4.5H2O was treated with an alk. soln. of NaBH4 and stirred for 3 h to give the activated catalyst. H2C:CHCN was treated with the Cu catalyst at a mol. ratio of 2:1, heated to 90° and maintained at this temp. for 2 h with vigorous shaking to give 94.6% H2C:CHCONH2, with a selectivity of 100%.

IT 100-54-9, Nicotinonitrile

RL: RCT (Reactant); RACT (Reactant or reagent) (hydration of, to amide, copper catalyst for)

RN 100-54-9 HCAPLUS

CN 3-Pyridinecarbonitrile (9CI) (CA INDEX NAME)

RN

IT 98-92-0P, Nicotinamide

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of, by hydration of nitrile, copper catalyst for) 98-92-0 HCAPLUS

CN 3-Pyridinecarboxamide (9CI) (CA INDEX NAME)



HCAPLUS COPYRIGHT 2003 ACS L15 ANSWER 4 OF 5

Citing References ACCESSION NUMBER:

1985:476789 HCAPLUS

DOCUMENT NUMBER:

103:76789

TITLE:

Study of the activity and selectivity of an supported

catalyst from oxides of metals of varying valence

in the oxidative ammonolysis of 3-picoline

AUTHOR (S):

Koshevnik, M. A.; German, E. N.; Guseinov, E. M.

CORPORATE SOURCE:

SOURCE:

Deposited Doc. (1984), VINITI 5036-84, 123-6 Avail.:

VINITI

DOCUMENT TYPE:

Report

LANGUAGE: Russian

The activity and selectivity of the com. catalyst KVTS (V and Ti oxides) and of newly prepd. catalyst K-3 were studied in oxidative ammonolysis of 3-picoline. The K-3 catalyst exhibits high activity and selectivity with 90-93% yield of nicotinic acid amide and nitrile at the total conversion of starting material. It allows 2-3 fold larger productivity of a reactor and decreases energy losses (related with the utilization of large amt. of steam with com. catalyst) as compared to the use of KVTS.

IT 98-92-0P 100-54-9P

RL: RCT (Reactant); PREP (Preparation); RACT (Reactant

or reagent)

(synthesis of, by oxidative ammonolysis of 3-picoline, activity and reactivity of catalysts for)

RN 98-92-0 HCAPLUS

3-Pyridinecarboxamide (9CI) (CA INDEX NAME) CN

RN 100-54-9 HCAPLUS

CN 3-Pyridinecarbonitrile (9CI) (CA INDEX NAME)

L15 ANSWER 5 OF 5 HCAPLUS COPYRIGHT 2003 ACS

Citing References Text

ACCESSION NUMBER: 1974:505297 HCAPLUS

DOCUMENT NUMBER:

81:105297

TITLE.

Pyridinecarboxylic acid amides

INVENTOR(S):

Watabiki, Yukio; Sugimoto, Nobutaka; Sakai, Koji; Miyoshi, Masamitsu; Uehara, Yoshihiro; Hakozaki,

Akiyoshi

PATENT ASSIGNEE(S):

Yuki Gosei Kogyo Co., Ltd.

Jpn. Kokai Tokkyo Koho, 5 pp.

DOCUMENT TYPE:

Patent

CODEN: JKXXAF

LANGUAGE:

SOURCE:

FAMILY ACC. NUM. COUNT:

Japanese

PATENT INFORMATION:

PATENT NO.

KIND DATE

APPLICATION NO. DATE <u>JP 49062474</u> A2 19740617 <u>JP 1972-103976</u> 19721019

JP 51006672 B4 19760301

<u>PRIORITY</u> APPLN. INFO.: <u>JP 1972-103976</u> 19721019

AB Pyridinecarboxylic acid amides were prepd. by hydrolysis of cyanopyridines in the presence of metal chromite catalysts comprising Cr and Cu (or Zn, Sn, Co, Mn, or Ni). Thus, refluxing a mixt. of 80 g 3-cyanopyridine (I) and 0.5 g Ni chromite catalyst in H2O 9 hr gave a product contg. 99.88 mole % (to I) nicotinamide. 4-Cyanopyridine was similarly converted to 98.68 mole % isonicotinamide by use of Cu chromite.

IT 98-92-0P

RL: PREP (Preparation)

(from hydrolysis of 3-cyanopyridine)

RN 98-92-0 HCAPLUS

CN 3-Pyridinecarboxamide (9CI) (CA INDEX NAME)

IT 100-48-1

RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrolysis of, isonicotinamide from)

RN 100-48-1 HCAPLUS

CN 4-Pyridinecarbonitrile (9CI) (CA INDEX NAME)

IT 100-54-9

RL: RCT (Reactant); RACT (Reactant or reagent) (hydrolysis of, nicotinamide from)

RN 100-54-9 HCAPLUS

CN 3-Pyridinecarbonitrile (9CI) (CA INDEX NAME)

=> file caold

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 29.44 204.41 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL SESSION ENTRY CA SUBSCRIBER PRICE -3.26 -3.26

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FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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(FILE 'HOME' ENTERED AT 05:20:39 ON 30 JUN 2003)

FILE 'REGISTRY' ENTERED AT 05:20:47 ON 30 JUN 2003

E NICOTINAMIDE/CN

L1 1 S E3

E CYANOPYRIDINE/CN

L2 1 S E3

L3 STRUCTURE UPLOADED

L4 50 S L3

L5 34801 S L3 FULL

L6 STRUCTURE UPLOADED

L7 18 S L6

FILE 'HCAPLUS' ENTERED AT 05:27:14 ON 30 JUN 2003

L8 250 S L1/PREP

L9 5151 S L5/RCT

L10 80 S L9 AND L8

FILE 'REGISTRY' ENTERED AT 05:28:15 ON 30 JUN 2003

E WATER/CN

L11 1 S E3

FILE 'HCAPLUS' ENTERED AT 05:28:39 ON 30 JUN 2003

L12 21445 S L11/RCT

L13 0 S L12 AND L10

L14 7 S L10 AND METAL?

L15 5 S L14 AND CATAL?

FILE 'CAOLD' ENTERED AT 05:30:18 ON 30 JUN 2003

=> s 11 and 15

TOO MANY TERMS FOR FILE CROSSOVER IN L5

There are limits on the size of an answer set being crossed over from one file to another. Enter <u>HELP CROSSOVER</u> at an arrow prompt (=>) for specific information.

=> s l1

L16 9 L1

=> s 15

TOO MANY TERMS FOR FILE CROSSOVER IN L5 . There are limits on the size of an answer set being crossed over from

one file to another. Enter HELP CROSSOVER at an arrow prompt (=>) for specific information.

=> s 12

1 L2 L17

=> s 11 and 12

9 L1

1 L2

L18 0 L1 AND L2

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SINCE FILE COST IN U.S. DOLLARS TOTAL ENTRY SESSION

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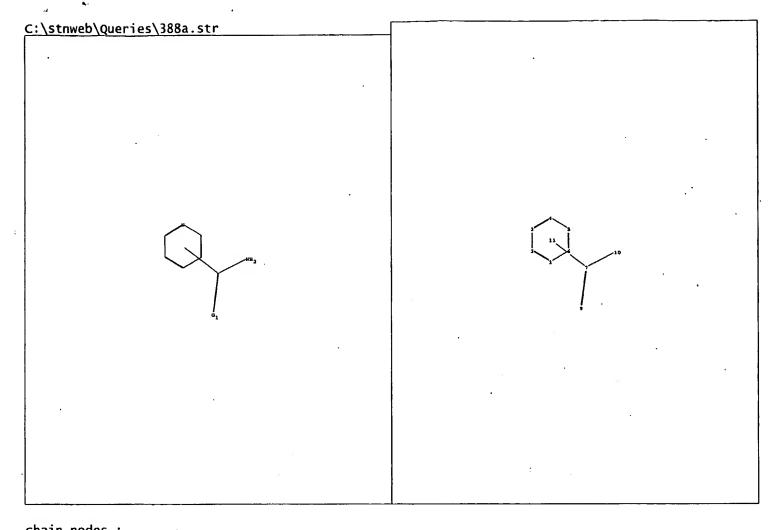
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STN INTERNATIONAL LOGOFF AT 05:31:36 ON 30 JUN 2003

C:\stnweb\Queries\388.str

chain nodes:
 7
ring nodes:
 1 2 3 4 5 6
ring bonds:
 1-2 1-6 2-3 3-4 4-5 5-6
normalized bonds:
 1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems:
 containing 1:

Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS



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chain nodes:
    7 9 10
ring nodes:
    1 2 3 4 5 6
chain bonds:
    7-9 7-10
ring bonds:
    1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds:
    7-9 7-10
normalized bonds:
    1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems:
    containing 1:
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G1:0,S

Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:CLASS 10:CLASS 11:CLASS